The Pfaffian solution of a dimer-monomer problem: Single monomer on the boundary

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We consider the dimer-monomer problem for the rectangular lattice. By mapping the problem into one of close-packed dimers on an extended lattice, we rederive the Tzeng-Wu solution for a single monomer on the boundary by evaluating a Pfaffian. We also clarify the mathematical content of the Tzeng-Wu solution by identifying it as the product of the nonzero eigenvalues of the Kasteleyn matrix.

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I. INTRODUCTION

An outstanding unsolved problem in lattice statistics is the dimer-monomer problem. While it is known [1] that the dimer-monomer system does not exhibit a phase transition, there have been only limited closed-form results. The case of close-packed dimers on planar lattices has been solved by Kasteleyn [2] and by Temperley and Fisher [3, 4], and the solution has been extended to nonorientable surfaces [5, 6]. But the general dimer-monomer problem has proven to be intractable [7].

In 1974 Temperley [8] pointed out a bijection between configurations of a single monomer on the boundary of a planar lattice and spanning trees on a related lattice. The bijection was used in [8] to explain why enumerations of close-packed dimers and spanning trees on square lattices yield the same Catalan constant. More recently Tzeng and Wu [9] made further use of the Temperley bijection to obtain the closed-form generating function for a single monomer on the boundary. The derivation is however indirect since it makes use of the Temperley bijection which obscures the underlining mathematics of the closed-form solution.

Motivated by the Tzeng-Wu result, there has been renewed interest in the general dimer-monomer problem. In a series of papers Kong [10, 11, 12] has studied numerical enumerations of such configurations on $m\times n$ rectangular lattices for varying m, n, and extracted finite-size correction terms for the single-monomer [10] and general monomer-dimer [11, 12] problems. Of particular interest is the finding [10] that in the case of a single monomer the enumeration exhibits a regular pattern similar to that found in the Kasteleyn solution of close-packed dimers. This suggests that the general single-monomer problem might be soluble.

As a first step toward finding that solution it is necessary to have an alternate and direct derivation of the Tzeng-Wu solution without the recourse of the Temperley bijection. Here we present such a derivation. Our new approach points to the way of possible extension toward the general single-monomer problem. It also identifies that, besides an overall constant, the Tzeng-Wu solution is given by the square root of the product of the nonzero eigenvalues of the Kasteleyn matrix, and thus clarifies its underlining mathematics.

II. THE SINGLE MONOMER PROBLEM

Consider a rectangular lattice $\mathcal{L}$ consisting of an array of M rows and N columns, where both M and N are odd. The lattice consists of two sublattices A and B. Since the total number of sites MN is odd, the four corner sites belong to the same sublattice, say, A and there are one more A than B sites. The lattice can therefore be completely covered by dimers if one A site is left open. The open A site can be regarded as a monomer.

Assign non-negative weights x and y respectively to horizontal and vertical dimers. When the monomer is on the boundary, Tzeng and Wu [9] obtained the following closed-form expression for the generating function,

$$G(x,y) = x^{(M-1)/2}y^{(N-1)/2} \times \prod_{m=1}^{\frac{M-1}{2}}\prod_{n=1}^{\frac{N-1}{2}}\left[4x^2\cos^2\frac{m\pi}{M+1}+4y^2\cos^2\frac{n\pi}{N+1}\right]. \quad (1)$$

This result is independent of the location of the monomer provided that it is on the boundary.

We rederive the result (1) using a formulation which is applicable to any dimer-monomer problem. We first expand $\mathcal{L}$ into an extended lattice $\mathcal{L}'$ constructed by connecting each site occupied by a monomer to a new added site, and then consider close-packed dimers on $\mathcal{L}'$. Since the newly added sites are all of degree 1, all edges originating from the new sites must be covered by dimers. Consequently, the dimer-monomer problem on $\mathcal{L}$ (with fixed monomer sites) is mapped to a close-packed dimer problem on $\mathcal{L}'$, which can be treated by standard means.

We use the Kasteleyn method [2] to treat the latter problem. Returning to the single-monomer problem let the boundary monomer be at site $s_0 = (1, n)$ as demonstrated in Fig. 1a. The site s_0 is connected to a new site s' by an edge with weight 1 as shown in Fig. 1b. To enumerate close-packed dimers on $\mathcal{L}'$ using the Kasteleyn approach, we need to orient, and associate phase factors

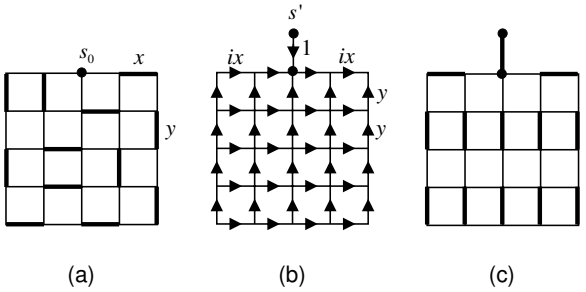

FIG. 1: (a) A dimer-monomer configuration on a 5×5 lattice $\mathcal{L}$ with a single monomer at $s_0=(1,3)$. (b) The extended lattice $\mathcal{L}'$ with edge orientation and a phase factor i to horizontal edges. (c) The reference dimer configuration C_0.

to, edges so that all terms in the resulting Pfaffian yield the same sign.

A convenient choice of orientation and assignment of phase factors is the one suggested by T. T. Wu [13]. While Wu considered the case MN = even, the consideration can be extended to the present case. Orient all horizontal (resp. vertical) edges in the same direction and the new edge from s' to s_0, and introduce a phase factor i to all horizontal edges as shown in Fig. 1b. Then all terms in the Pfaffian assume the same sign. To prove this assertion it suffices to show that a typical term in the Pfaffian associated with a dimer configuration C has the same sign as the term associated with a reference configuration C_0. For C_0 we choose the configuration shown in Fig. 1c, in which horizontal dimers are placed in the first row with vertical dimers covering the rest of the lattice. Then C and C_0 assume the same sign.

The simplest way to verify the last statement is to start from a configuration in which every heavy edge in C_0 shown in Fig. 1c is occupied by two dimers, and view each of the doubly occupied dimers as a polygon of two edges. Then the 'transposition polygon' (Cf. [2]) formed by superimposing any C and C_0 can always be generated by deforming some of the doubly occupied edges into bigger polygons, a process which does not alter the overall sign. It follows that C and C_0 have the same sign for any C. This completes the proof.

Here we have implicitly made use of the fact that the monomer is on the boundary. If the monomer resides in the interior of $\mathcal{L}$, then there exist transposition polygons encircling the monomer site which may not necessarily carry the correct sign. The Pfaffian, while can still be evaluated, does not yield the dimer-monomer generating function. We shall consider this general single-monomer problem subsequently [14].

With the edge orientation and phase factors in place, the dimer generating function G is obtained by evaluating a Pfaffian

$$G(x,y)=\mathrm{Pf}(A')=\sqrt{\mathrm{Det}\ A'} \tag{2}$$

where A' is the antisymmetric Kasteleyn matrix of dimension $(MN+1)\times(MN+1)$. Explicitly, it reads

$$A'=\begin{pmatrix} 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & & & & & & & \\ \vdots & & & & & & & \\ 0 & & & & & & & \\ -1 & & & & A & & & \\ 0 & & & & & & & \\ \vdots & & & & & & & \\ 0 & & & & & & & \end{pmatrix}. \tag{3}$$

Here, A is the Kasteleyn matrix of dimension MN for $\mathcal{L}$ given by

$$A=i\,x\,T_M\otimes I_N+y\,I_M\otimes T_N, \tag{4}$$

with I_N the $N\times N$ identity matrix and T_N the $N\times N$ matrix

$$T_N=\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \ldots & 0 & 1 \\ 0 & 0 & 0 & \ldots & -1 & 0 \end{pmatrix}. \tag{5}$$

Note that elements of A are labeled by $\{(m,n);(m',n')\}$, where (m,n) is a site index, and the element 1 in the first row of A' is at position $(1,n)$ of A, $n=$ odd.

Expanding (3) along the first row and column, we obtain

$$\mathrm{Det}\,A'=C(A;\{(1,n);(1,n)\}) \tag{6}$$

where $C(A;\{(1,n);(1,n)\})$ is the cofactor of the $\{(1,n);(1,n)\}$-th element of Det A.

The cofactor $C(\alpha,\beta)$ of the (α,β)-th element of any non-singular A can be computed using the identity

$$C(A;\alpha,\beta)=A^{-1}(\beta,\alpha)\times\mathrm{Det}\,A, \tag{7}$$

where $A^{-1}(\beta,\alpha)$ is the (β,α)-th element of A. However, the formula is not directly useful in the present case since the matrix A is singular. We shall return to its evaluation in Sec. IV.

III. EIGENVALUES OF THE DETERMINANT A

In this section we enumerate the eigenvalues of A.

The matrix T_N is diagonalized by the similarity transformation

$$U_N^{-1}\,T_N\,U_N=\Lambda_N$$

where U_N and U_N^{-1} are $N\times N$ matrices with elements

$$\begin{aligned} U_N(n_1,n_2) &= \sqrt{\frac{2}{N+1}}\,i^{\,n_1}\sin\frac{n_1n_2\pi}{n+1} \\ U_N^{-1}(n_1,n_2) &= \sqrt{\frac{2}{N+1}}\,(-i)^{n_2}\sin\frac{n_1n_2\pi}{N+1}, \end{aligned} \tag{8}$$

and Λ_N is an $N \times N$ diagonal matrix whose diagonal elements are the eigenvalues of T_N,

$$\lambda_m = 2i \cos \frac{m\pi}{N+1}, \quad m = 1, 2, \cdots, N. \tag{9}$$

Similarly the $MN \times MN$ matrix A is diagonalized by the similarity transformation generated by $U_{MN} = U_M \otimes U_N$. Namely,

$$U_{MN}^{-1} A U_{MN} = \Lambda_{MN} \tag{10}$$

where Λ_{MN} is a diagonal matrix with eigenvalues

$$\begin{aligned} l_{mn} &= 2i\left[i\, x \cos \frac{m\pi}{M+1} + y \cos \frac{n\pi}{N+1}\right], \\ & m = 1, 2, ..., M,\ n = 1, 2, ..., N, \end{aligned} \tag{11}$$

on the diagonal, and elements of U_{MN} and U_{MN}^{-1} are

$$\begin{aligned} U_{MN}(m_1, n_1; m_2, n_2) &= U_M(m_1, m_2)\, U_N(n_1, n_2) \\ U_{MN}^{-1}(m_1, n_1; m_2, n_2) &= U_M^{-1}(m_1, m_2)\, U_N^{-1}(n_1, n_2). \end{aligned}$$

Then we have

$$\mathrm{Det}\, A = \prod_{m=1}^{M} \prod_{n=1}^{N} l_{mn}. \tag{12}$$

As in (2), close-packed dimers on $\mathcal{L}$ are enumerated by evaluating $\sqrt{\mathrm{Det} A}$. For MN even, this procedure gives precisely the Kasteleyn solution [2]. For MN odd, the case we are considering, the eigenvalue $l_{mn} = 0$ for $m = (M+1)/2, n = (N+1)/2$, and hence $\mathrm{Det}\, A = 0$, indicating correctly there is no dimer covering of $\mathcal{L}$. However, it is useful for later purposes to consider the product of the nonzero eigenvalues of A,

$$P \equiv \prod_{m=1}^{M} \prod_{n=1}^{N}{}' l_{mn}, \tag{13}$$

where the prime over the product denotes the restriction $(m, n) \neq (\frac{M+1}{2}, \frac{N+1}{2})$.

Using the identity

$$\cos\left(\frac{m}{M+1}\right)\pi = -\cos\left(\frac{M-m+1}{M+1}\right)\pi,$$

one can rearrange factors in the product to arrive at

$$P = Q \prod_{m=1}^{\frac{M-1}{2}} \prod_{n=1}^{\frac{N-1}{2}} \left(4x^2 \cos^2 \frac{m\pi}{M+1} + 4y^2 \cos^2 \frac{n\pi}{N+1}\right)^2 \tag{14}$$

where the factor Q is the product of factors with either $m = \frac{M+1}{2}$ or $n = \frac{N+1}{2}$. Namely,

$$\begin{aligned} Q &= \left[\prod_{m=1}^{\frac{M-1}{2}} 4x^2 \cos^2 \frac{m\pi}{M+1}\right] \times \left[\prod_{n=1}^{\frac{N-1}{2}} 4y^2 \cos^2 \frac{n\pi}{N+1}\right] \\ &= \left[\frac{(M+1)(N+1)}{4}\right] x^{M-1} y^{N-1}, \end{aligned} \tag{15}$$

where we have made use of the identity

$$\prod_{n=1}^{\frac{N-1}{2}} \left(4 \cos^2 \frac{n\pi}{N+1}\right) = \frac{N+1}{2}, \quad N = \text{odd}.$$

The expression (14) for P will be used in the next section.

IV. EVALUATION OF THE COFACTOR

We now return to the evaluation of the cofactor $C(A; \{(1, n); (1, n)\})$. We shall however evaluate the cofactor $C(A; \{(m, n); (m', n')\})$ for general m, m', n, n', although only the result of $m = m' = 1$, $n = n'$ is needed here.

To circumvent the problem of using (7) caused by the vanishing of $\mathrm{Det}\, A = 0$, we replace A by the matrix

$$A(\epsilon) = A + \epsilon\, I_{MN}, \quad \epsilon \neq 0$$

whose inverse exists, and take the $\epsilon \to 0$ limit to rewrite (7) as

$$\begin{aligned} &C(A; \{(m, n); (m', n')\}) \\ &\quad = \lim_{\epsilon \to 0} \Big[\big[A^{-1}(\epsilon)\big](m', n'; m, n) \times \mathrm{Det}\ A(\epsilon)\Big]. \end{aligned} \tag{16}$$

Quantities on the r.h.s. of (16) are now well-defined and the cofactor can be evaluated accordingly. The consideration of the inverse of a singular matrix along this line is known in mathematics literature as finding the pseudo-inverse [15, 16]. The method of taking the small ϵ limit used here has previously been used successfully in the analyses of resistance [17] and impedance [18] networks.

The eigenvalues of $A(\epsilon)$ are $l_{mn}(\epsilon) = l_{mn} + \epsilon$ and hence we have

$$\mathrm{Det}\, A(\epsilon) = \prod_{m=1}^{M} \prod_{n=1}^{N} \big[l_{mn} + \epsilon\big] = \epsilon\, P + O(\epsilon^2), \tag{17}$$

where P is the product of nonzero eigenvalues given by (14).

We next evaluate $A^{-1}(\epsilon)(m.n; m, n)$ and retain only terms of the order of $1/\epsilon$. Taking the inverse of (10) with $A(\epsilon)$ in place of A, we obtain

$$A^{-1}(\epsilon) = U_{MN}\, \Lambda_{MN}^{-1}(\epsilon)\, U_{MN}^{-1}.$$

Writing out its matrix elements explicitly, we have

$$A^{-1}(\epsilon)(m',n';m,n) = \sum_{m''=1}^{M}\sum_{n''=1}^{N} \frac{U_{MN}(m',n';m'',n'')U^{-1}_{MN}(m'',n'';m,n)}{l_{m'',n''}+\epsilon}. \tag{18}$$

For ϵ small the leading term comes from $(m'',n'') = (\frac{M+1}{2}, \frac{N+1}{2})$ for which $l_{m'',n''} = 0$. Using $U^{-1}_{MN}(m,n;m',n') = U^{-1}_{M}(m,m')\,U^{-1}_{N}(n,n')$ and (8), this leads to the expression

$$A^{-1}(\epsilon)(m',n';m,n) \;=\; \left(\frac{1}{\epsilon}\right)\left[\frac{4\,i^{m'+n'}(-i)^{m+n}}{(M+1)(N+1)}\right]\sin\frac{m'\pi}{2}\sin\frac{n'\pi}{2}\sin\frac{m\pi}{2}\sin\frac{n\pi}{2} + \; O(1).$$

Thus, after making use of (16) and (17) we obtain

$$\begin{aligned} &C(A;\{(m,n);(m',n')\}) \\ &= \sin\frac{m\pi}{2}\sin\frac{n\pi}{2}\sin\frac{m'\pi}{2}\sin\frac{n'\pi}{2}\left[\frac{4\,i^{m'+n'}(-i)^{m+n}P}{(M+1)(N+1)}\right]. \end{aligned} \tag{19}$$

Finally, specializing to $m = m' = 1$, $n = n'$ and combining (2), (6), and (19), we obtain

$$\begin{aligned} G(x,y) \;&=\; \sqrt{C(A;\{(1,n);(1,n)\})} \\ &=\; \sqrt{\frac{4P}{(M+1)(N+1)}}, \quad \text{for } n \text{ odd } (A \text{ site}) \\ &=\; 0, \qquad\qquad\qquad\quad \text{for } n \text{ even } (B \text{ site}) \end{aligned} \tag{20}$$

This gives the result (1) after introducing (14) for P. It also says that there is no dimer covering if the monomer is on a B site.

The expression (20) clarifies the underlining mathematical content of the Tzeng-Wu solution (1) by identifying it as the product of the *nonzero* eigenvalues of the Kasteleyn matrix. This is compared to the Kasteleyn result [2] that for $MN =$ even the dimer generating function is given by the product of *all* eigenvalues.

V. DISCUSSIONS

We have used a direct approach to derive the closed-form expression of the dimer-monomer generating function for the rectangular lattice with a single monomer on the boundary. Our approach is to first convert the problem into one of close-packed dimers without monomers, and consider the latter problem using established means. This approach suggests a possible route toward analyzing the general dimer-monomer problem.

We have also established that the Tzeng-Wu solution (1) is given by the product of the nonzero eigenvalues of the Kasteleyn matrix of the lattice. This is reminiscent to the well-known result in algebraic graph theory [19] that spanning trees on a graph are enumerated by evaluating the product of the nonzero eigenvalues of its tree matrix. The method of evaluating cofactors of a singular matrix as indicated by (16), when applied to the tree matrix of spanning trees details of which can be easily worked out, offers a simple and direct proof of the fact that all cofactors of a tree matrix are equal and equal to the product of its nonzero eigenvalues. The intriguing similarity of the results suggests there might be something deeper lurking behind our analysis.

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